



# Predictive Engineering Tools for Injection-Molded Long Carbon Fiber Thermoplastic Composites

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PNNL-SA-125243

Project ID# LM116

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# Overview

## Timeline

- **Start:** September 2012
- **End:** July 2017
- **Percent complete:** 99%

## Budget

- **Total project:** \$2.1M
  - DOE: \$1.0M (received FY12)
  - Cost share: \$1.1M (52%)
- **Expenditures through FY16:**
  - DOE: \$994k
  - Cost share: \$1.4M (58%)
- **FY 2017 funding**
  - DOE share: \$6.5k (carried over)

## Barriers addressed

- **Manufacturability:** it is difficult to injection mold highly loaded ( $\geq 50\text{wt}\%$ ) long carbon fiber ( $> 2\text{mm}$ ) thermoplastics (LCFTs)
- **Predictive tools:** LCFT models need development/validation

## Partners

- PNNL (Lead)
- Autodesk, Inc.
- Toyota Research Institute N. America
- MAGNA Exteriors & Interiors Corp.
- PlastiComp, Inc.
- Purdue University
- Virginia Polytechnic & State University
- Univ. of Illinois at Urbana-Champaign

# Project Objectives/Relevance

## Overall Objective

- Optimize/validate previously developed predictive engineering (PE) tools to predict fiber orientation (FO) and length distributions (FLD) in complex\* three-dimensional (3D) automotive parts injection molded from long carbon fiber (LCF)-reinforced polypropylene and polyamide-6,6 compounds

\*Complex = shape must cause a change flow direction and thickness in the mold and be a prototype for lightweighting the Body system (DE-FOA-0000648, AOI1)

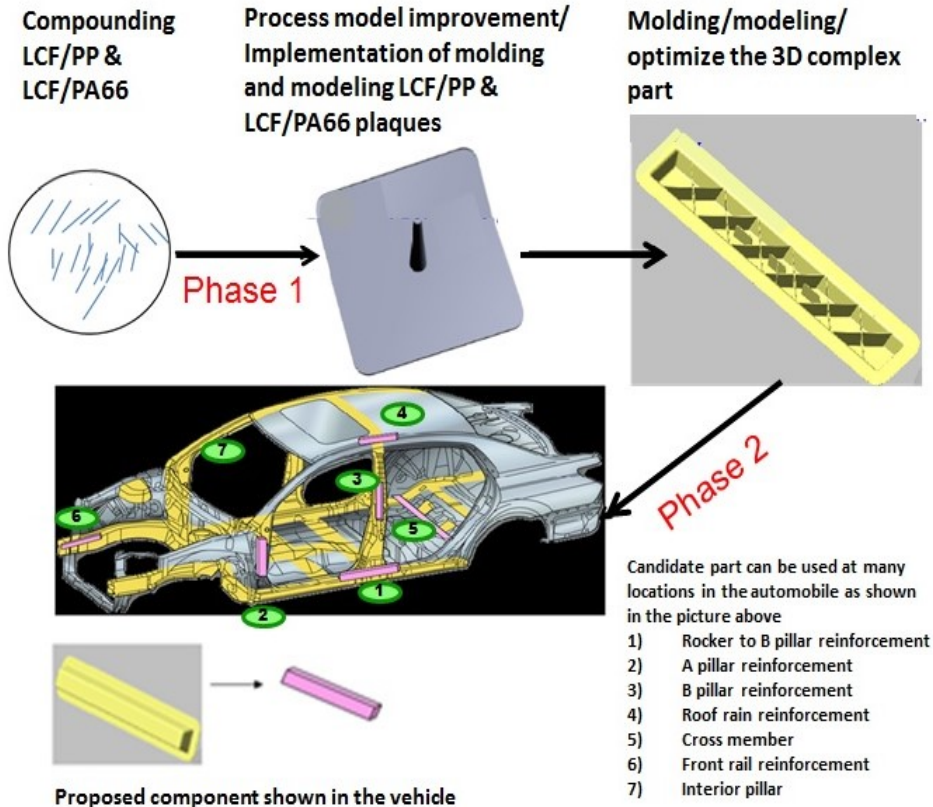
## Specific Objectives

- Ph1: Predict FO & FLD in 2D plaques within 15% of experimental results
- Ph2: Predict FO & FLD in 3D complex parts w/i 15% of experimental results
- Estimate cost/weight savings achievable for vehicle body system

## Impact

- Optimized and validated PE tools that predict system performance from process and design variables help facilitate use of lightweighting technologies with resulting decrease in energy usage and emissions

# Approach



- ASMI = Autodesk® Simulation Moldflow® Insight (Autodesk.com)
- EMTA = Eshelby-Mori-Tanaka Approach
- EMTA-NLA = Eshelby-Mori-Tanaka Approach to Non-Linear Analysis

- ▶ Build on prior PE efforts for long glass fiber thermoplastic composites (ASMI, EMTA, EMTA-NLA) to validate the PE tools for injection-molded LCFTs
- ▶ Predict fiber orientation (FO) and fiber length distribution (FLD) in molded parts from injection molding conditions and compare predictions to measured data
- ▶ Calculate stiffness using FO and FLD values to evaluate prediction accuracy
- ▶ Use calculated stiffness performance and industrial partners' inputs to estimate potential for weight and cost savings in vehicle body system using long carbon fiber injection molded thermoplastic technology

# Schedule and Milestones

Task	FY14	FY15	FY16
ASMI Model Integration	Autodesk/UIUC		
LCF/PP & LCF/PA66 Compounding	PlastiComp		
Plaque Molding	PlastiComp		
Compound Testing	Autodesk		
Plaque Process Modeling	PNNL/UIUC/Autodesk		
Plaque Fiber Measurement	Purdue		
<b>Go/No Go: Validate Tools for Plaques</b>			★
Complex Part Molding	PlastiComp/Magna		
Part Process Modeling	PNNL/UIUC/Autodesk		
Part Fiber Measurement	Virginia Tech		
Weight/Cost Analysis	PNNL/Toyota/Magna/PlastiComp		

\* ASMI = Autodesk® Simulation Moldflow® Insight, LCF = long carbon fiber, PP = polypropylene, PA66 = polyamide-6,6

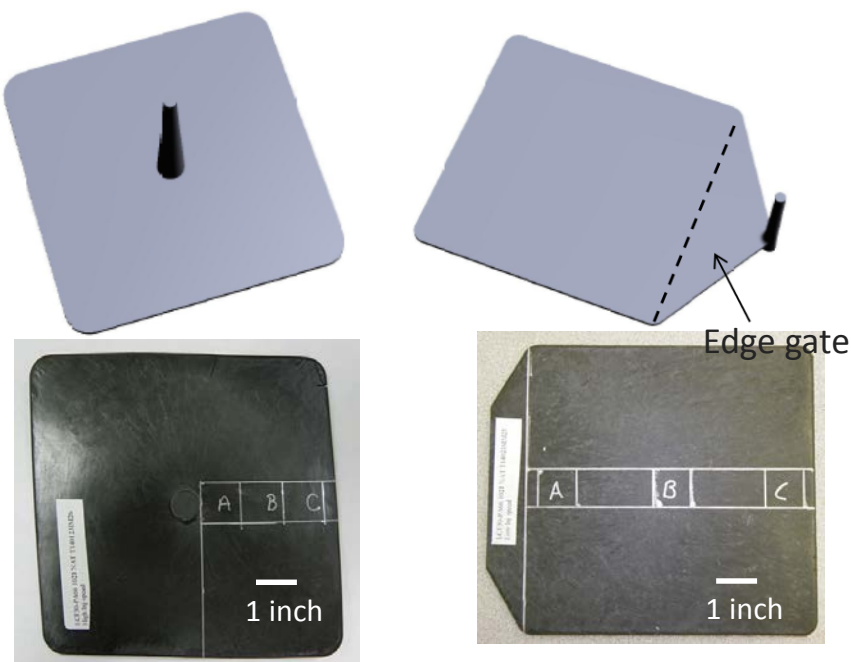
# Technical Accomplishments Summary

- ▶ Pellets compounded, plaques molded
  - LCF/PP, LCF/PA66, 30%, 50%, Fast, Slow, Edge, Center
- ▶ FO and FLD for plaques measured, simulated (2D & 3D models)
- ▶ Tensile/flexural stiffness computed from measured FO & FLD values and from predicted values to assess prediction accuracy
- ▶ Model accuracy improved, computational burden reduced
- ▶ Complex parts molded: Ribbed, Non-ribbed, 30wt%LCF/PP, /PA66
- ▶ FO and FLD for parts measured, simulated (2D & 3D models)
- ▶ Tensile/flexural stiffness computed for prediction assessment
- ▶ Potential weight savings and cost impact estimated

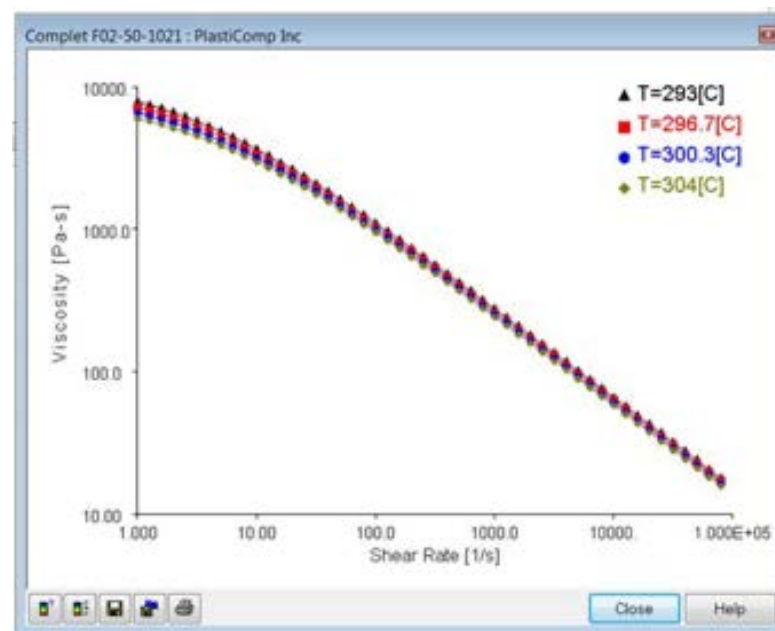
**Conclusion:** Predictive Engineering Tools validated for FO and FLD prediction enabling complex part long carbon fiber reinforced thermoplastics stiffness-based design

# Pellet, Plaque Production and Material Characterization

- ▶ **PlastiComp** produced compounds of 30wt% and 50wt% LCF in PP and PA66
- ▶ **PlastiComp** molded edge- and center-gated 7"x7"x1/8" plaques



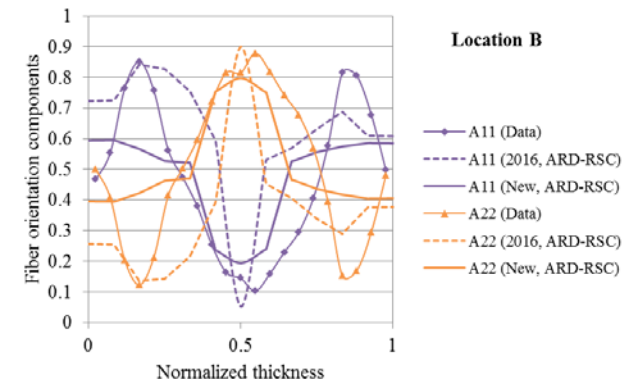
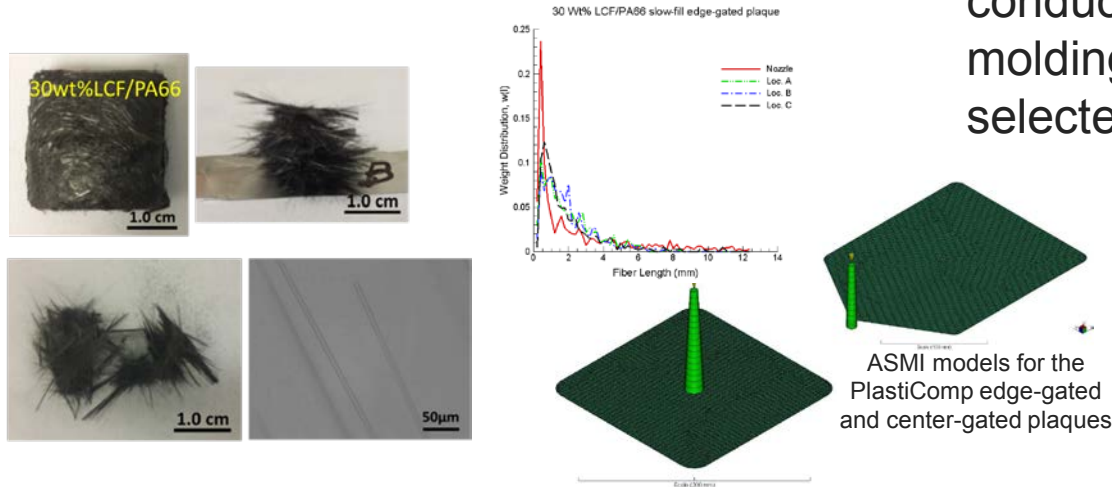
- ▶ **Autodesk** characterized the four compound variations for
  - Viscosity, Thermal Properties, Mechanical Properties, PVT / Density





# Fiber Measurement and Model Development

- ▶ **Purdue** developed/validated FO measurement method based on the principles of Univ. of Leeds method
- ▶ Developed partly automated method to measure FLD on **PNNL**-isolated fibers
- ▶ Measured FO/FLD on **PlastiComp** plaques at locations A, B, and C
- ▶ **Autodesk** improved ARD-RSC model accuracy, explored solution to capture the transverse alignment in core, and implemented ROM-POD, decreasing computation time and reducing memory for FLD calculation by 61%
- ▶ **PNNL**, with **Autodesk** and **UIUC**, conducted mid-plane & 3D ASMI injection molding analyses of **PlastiComp** plaques selected for the Go/No-go decision



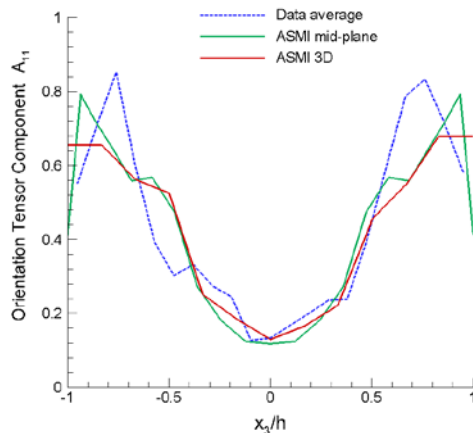
\*FO = fiber orientation, FLD = fiber length distribution, ASMI = Autodesk® Simulation Moldflow® Insight, ARD-RSC = anisotropic rotary diffusion – reduced strain closure, ROM-POD = reduced order model using proper orthogonal decomposition,



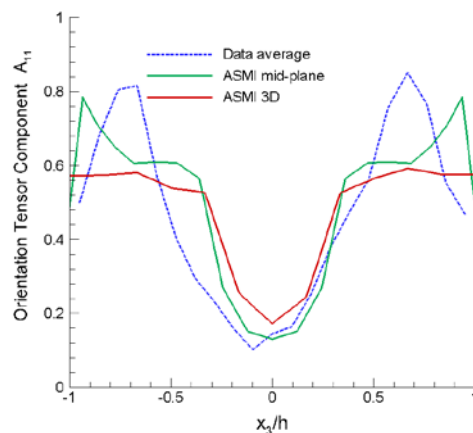
# Fiber Predictions & Measurements: Plaques

FO results for slow-fill 50wt% LCF/PP edge-gated plaque ( $A_{11}$ )

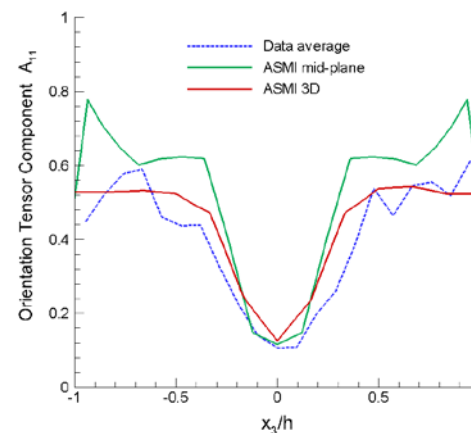
Fiber Orientation



**Location A**



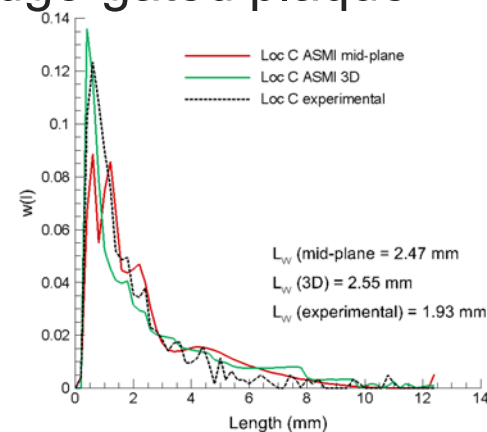
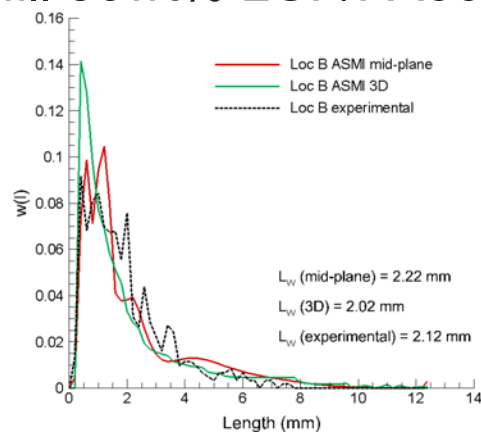
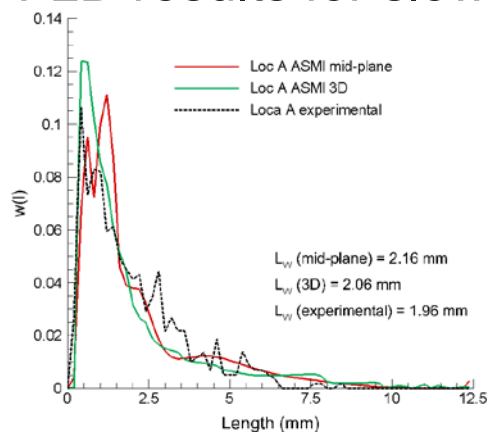
**Location B**



**Location C**

FLD results for slow-fill 30wt% LCF/PA66 edge-gated plaque

Fiber Length

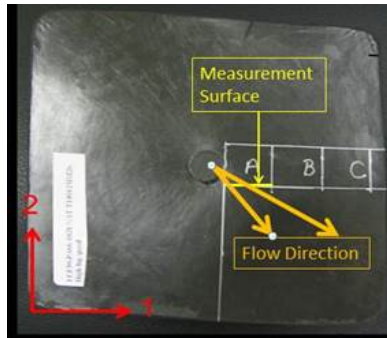


\*FO = fiber orientation, FLD = fiber length distribution

**Accuracy criterion met in 95% of  
FO cases, 100% of FLD cases**

# Prediction Validation for Plaques: the Go/No-go

- ▶ Tensile ( $E$ ) and Flexural ( $D$ ) moduli were computed from FO and FLD values at each plaque location (using EMTA) (A, B, C)
- ▶ Moduli based on predicted values were compared to moduli based on measured values to see if the  $\leq 15\%$  difference criterion was met
- ▶ 15% accuracy criterion met for
  - FO: 95% of cases for plaques
  - FLD: 100% of cases for plaques



\* EMTA = Eshelby-Mori-Tanaka Approach, FO = fiber orientation, FLD = fiber length distribution

Results illustrated for the slow-fill 50wt% LCF/PP edge-gated plaque

Tensile Modulus	$E_{11}$ (mid-plane FO) MPa	$E_{11}$ (3D FO) MPa	$E_{11}$ (measured FO) MPa	Agreement between 3D and measured
Loc. A	30371	29077	28984	0.32%
Loc. B	34736	30257	31425	3.72%
Loc. C	35965	26596	24672	7.80%
Tensile Modulus	$E_{22}$ (mid-plane FO) MPa	$E_{22}$ (3D FO) MPa	$E_{22}$ (measured FO) MPa	Agreement between 3D and measured
Loc. A	36083	36054	36153	0.27%
Loc. B	30179	31599	33704	6.25%
Loc. C	28394	34481	37095	7.05%
Flexural Modulus	$D_{11}$ (mid-plane FO) MPa.mm <sup>3</sup>	$D_{11}$ (3D FO) MPa.mm <sup>3</sup>	$D_{11}$ (measured FO) MPa.mm <sup>3</sup>	Agreement between 3D and measured
Loc. A	121362	120868	126761	4.65%
Loc. B	129217	109921	125239	12.23%
Loc. C	130646	98981	100300	1.32%
Flexural Modulus	$D_{22}$ (mid-plane FO) MPa.mm <sup>3</sup>	$D_{22}$ (3D FO) MPa.mm <sup>3</sup>	$D_{22}$ (measured FO) MPa.mm <sup>3</sup>	Agreement between 3D and measured
Loc. A	78584	71648	70924	1.02%
Loc. B	69276	78376	70755	10.77%
Loc. C	66765	86960	88048	1.24%

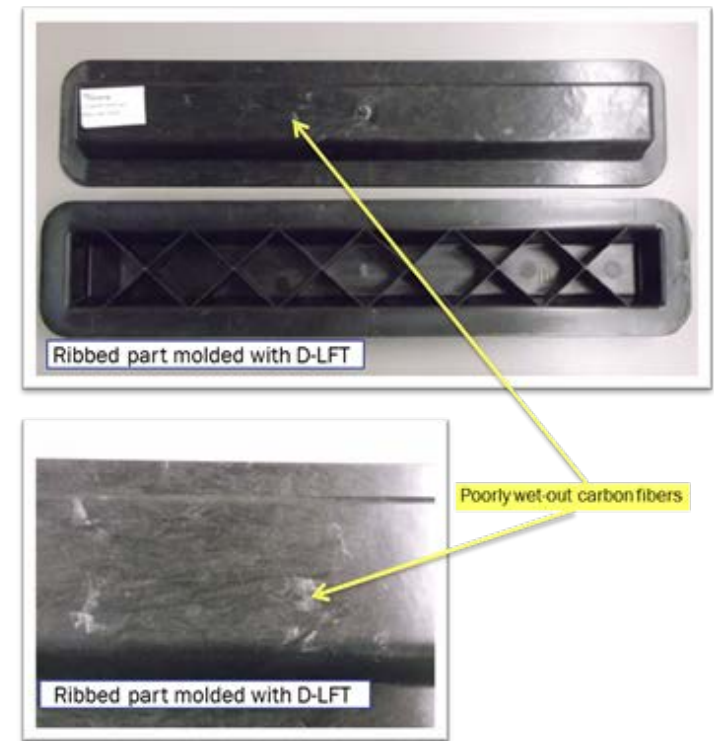
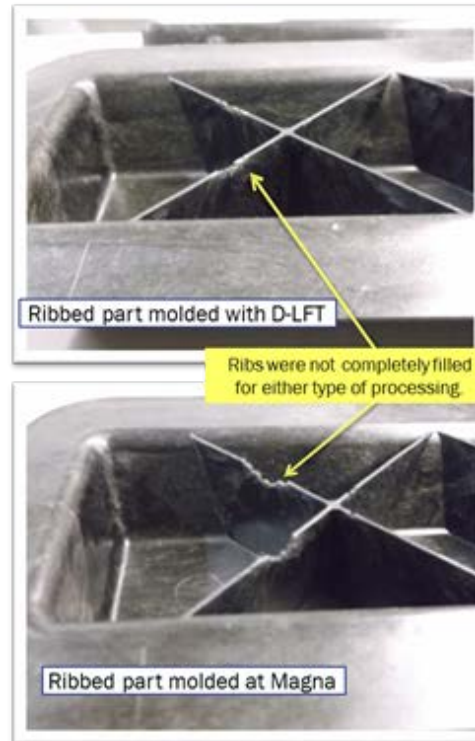
**Tool success in Phase 1-plaques enables transition to Phase 2-complex parts**

# Complex Part Molding

- ▶ **Magna** prepared tool with input from **Toyota & PlastiComp**
- ▶ 30wt%LCF/PP and 30%LCF/PA66, ribbed and non-ribbed parts
- ▶ **Magna** used Conventional LFT Molding, **PlastiComp** used D-LFT Pushtrusion®
- ▶ Non-ribbed parts molded very well, Ribs experienced incomplete filling
- ▶ D-LFT PP parts surfaces revealed poor wet-out at high fiber loading

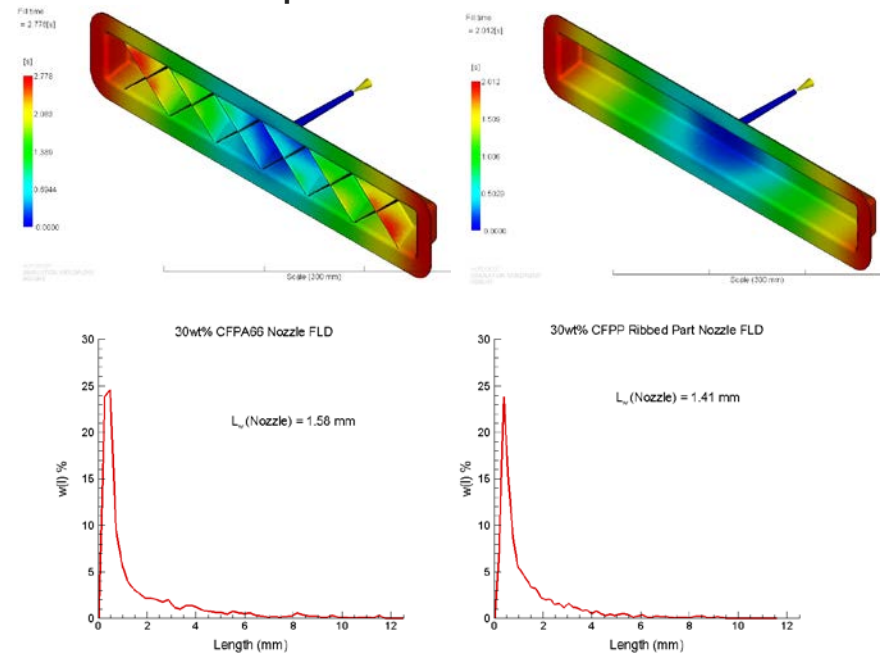
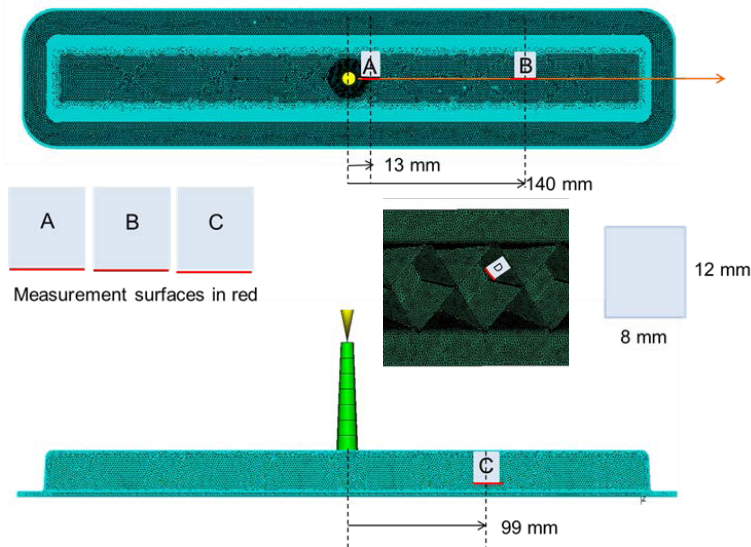


Short shot fill profiles



# Fibers in Complex Parts

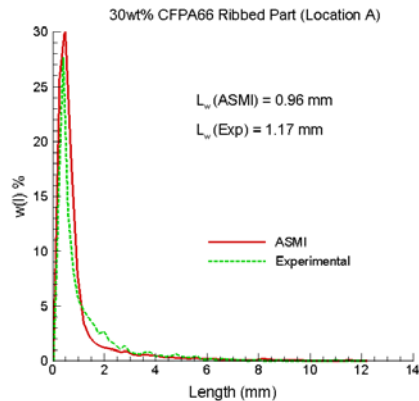
- ▶ **Magna** cut samples from the ribbed and non-ribbed parts at selected locations (A,B, C & D)
- ▶ **Virginia Tech** measured FO and FLD using existing protocols
- ▶ **PNNL & Autodesk** built 3D ASMI models for ribbed and non-ribbed parts using **Magna** parameters
- ARD-RSC model for FO prediction
- Phelps (2009) fiber breakage model for FLD prediction



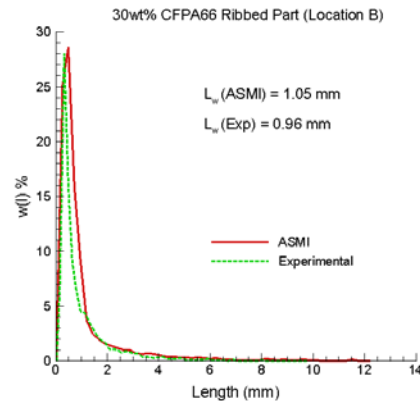
\*FO = fiber orientation, FLD = fiber length distribution, ASMI = Autodesk® Simulation Moldflow® Insight,  
 ARD-RSC = anisotropic rotary diffusion – reduced strain closure

# Fiber Predictions & Measurements: Complex Parts

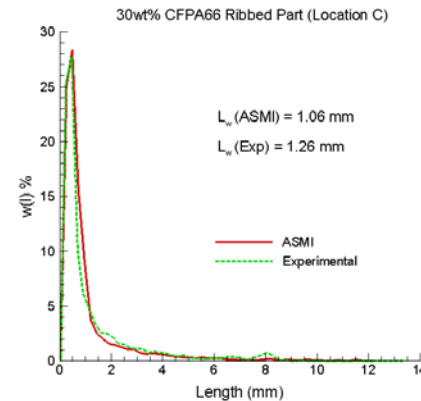
Results illustrated for the 30wt% LCF/PA66 ribbed part



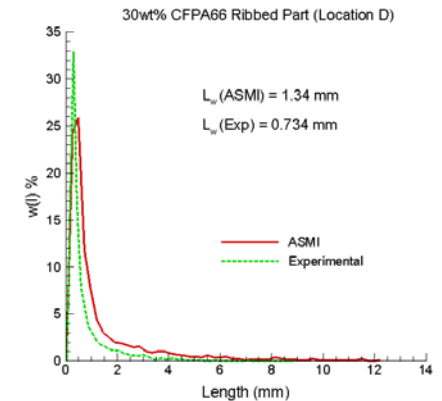
**Location A**



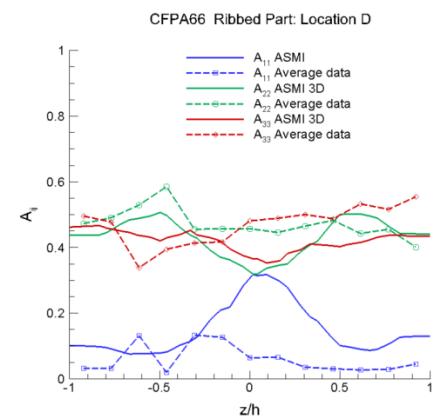
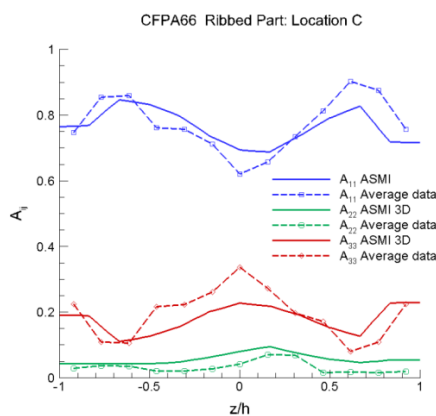
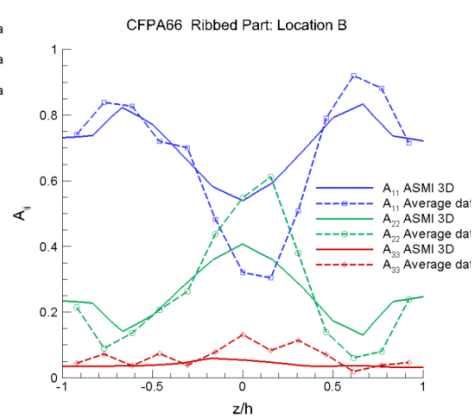
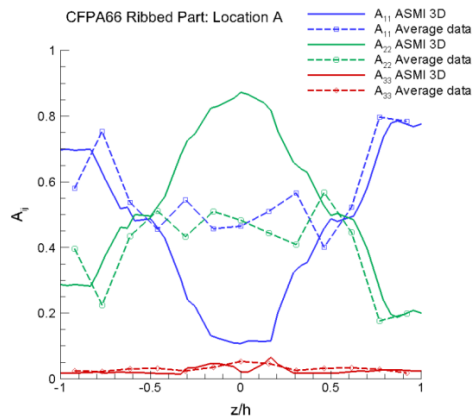
**Location B**



**Location C**



**Location D**



**Accuracy criterion met in 88% of  
FO cases, 100% of FLD cases**



# Prediction Validation for Complex Parts

- ▶ Tensile ( $E$ ) and Flexural ( $D$ ) moduli were computed from FO and FLD values at each part location (using EMTA) (A, B, C, D)
- ▶ Moduli based on predicted values were compared to moduli based on measured values to see if the  $\leq 15\%$  difference criterion was met
- ▶ 15% accuracy criterion met for: FO: 88% of part locations, FLD: 100% of locations

Results illustrated for the 30wt% LCF/PA66 ribbed part

Modulus (Location A)	Using Predicted Fiber Orientation	Using Measured Fiber Orientation	Agreement within
$E_{11}$ (MPa)	21134	25568	17.3%
$E_{22}$ (MPa)	24539	17585	39.5%
$D_{11}$ (MPa.mm <sup>3</sup> )	61510	62631	1.79%
$D_{22}$ (MPa.mm <sup>3</sup> )	34181	32747	4.38%

Modulus (Location B)	Using Predicted Fiber Orientation	Using Measured Fiber Orientation	Agreement within
$E_{11}$ (MPa)	33249	32268	3.04%
$E_{22}$ (MPa)	11795	12604	6.42%
$D_{11}$ (MPa.mm <sup>3</sup> )	73694	77610	5.05%
$D_{22}$ (MPa.mm <sup>3</sup> )	23568	20687	13.9%

Modulus (Location C)	Using Predicted Fiber Orientation	Using Measured Fiber Orientation	Agreement within
$E_{11}$ (MPa)	36280	37149	2.34%
$E_{33}$ (MPa)	8672	9982	13.1%
$D_{11}$ (MPa.mm <sup>3</sup> )	76774	80489	4.62%
$D_{33}$ (MPa.mm <sup>3</sup> )	20509	20754	1.18%

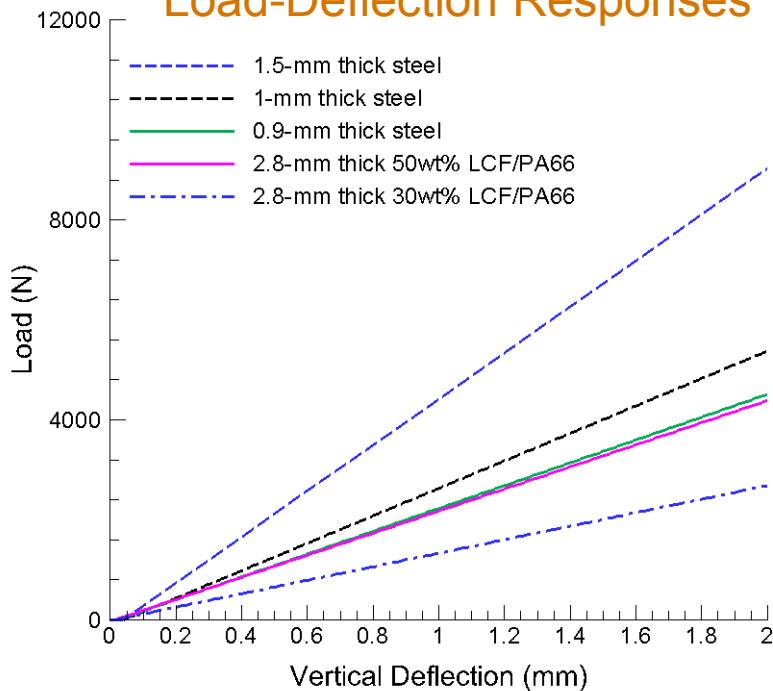
Modulus (Location D)	Using Predicted Fiber Orientation	Using Measured Fiber Orientation	Agreement within
$E_{22}$ (MPa)	16812	19849	15.3%
$E_{33}$ (MPa)	16390	20009	18.1%
$D_{22}$ (MPa.mm <sup>3</sup> )	3760	3977	5.46%
$D_{33}$ (MPa.mm <sup>3</sup> )	3641	4183	13.0%

\* EMTA = Eshelby-Mori-Tanaka Approach, FO = fiber orientation, FLD = fiber length distribution

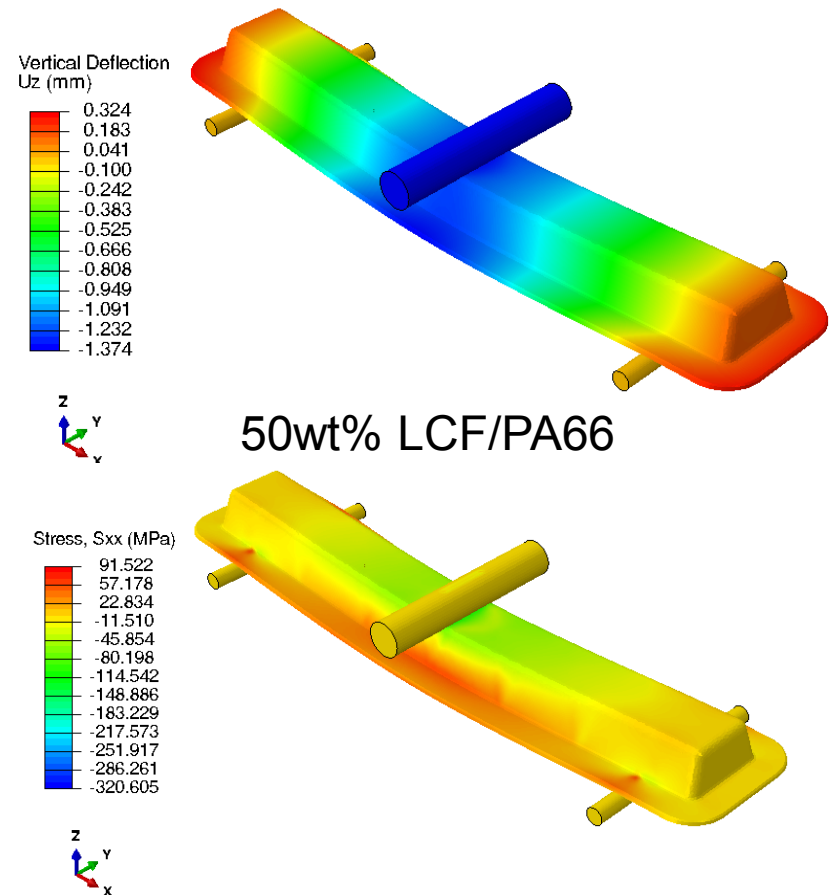
# Complex Part Bending Analysis for Weight Reduction Study

- ▶ PNNL's EMTA-NLA imported fiber orientation and length results from ASMI to ABAQUS enabling 3-point bending analyses of the complex ribbed parts

## Load-Deflection Responses



Stamped steel parts require thickness  $\geq 1\text{mm}$



\* EMTA-NLA = Eshelby-Mori-Tanaka Approach to Non-Linear Analysis, ASMI = Autodesk® Simulation Moldflow® Insight



# Body System Weight / Cost Reduction

## ► 50wt% LCF/PA66

- 43% weight reduction is possible for the considered complex part.
- Not all body system parts can be replaced with injection molded material.
- Practical manufacturing considerations were included in the weight analysis.

## ► The cost and weight impact on replacing steel parts with composite parts are:

Vehicle system	System definition	Weight reduction	Cost per lb saved	Additional requirements
Targets	Body in white, closures, fenders, bumpers	≥35%	< \$3.18/lb	Safety = OK Structure = OK
Results	Body in white + Closures	22.5 %	~ 5 times Target	Safety = NA Structure = OK
(if CF=\$5/lb)	Body in white + Closures	Same	2.5 times Target	Same

- Current estimate based on weight savings in BIW + closures and bumpers only.
- Lighter BIW can result in lighter secondary components (engine, brakes, suspension), multiplying opportunity for weight savings.
- The components whose main contribution is stiffness (bending) related are considered for weight saving replacement. The components playing significant role in the impact performance are not considered in the scope of this project.

# Response to Previous Year Reviewers' Comments (from 2014 AMR)

## **Regarding selection of materials and standardized material properties:**

- ▶ Material grades were selected by PlastiComp in the context of Magna and Toyota production-applicable considerations
- ▶ Calibration/verification of FO and FLD measurements were done using previously published FO data and LCF pellet dimensions
- ▶ Model includes material-specific properties
- ▶ Project evaluated LFT and D-LFT for injection molding of discontinuous fibers

## **Regarding integration of plaque and complex part phases**

- ▶ Prediction of molding of the part in Phase 1 following plaque experience informed the molding plan design for Phase 2, including changes to planned part wall thickness
- ▶ EMTA is the tie between FO, FLD and mechanical properties

## **Regarding reaching steady state flow**

- ▶ It is true that “small” (7”x7”) plaques may not be sufficient to capture steady state flow field in flow and cross-flow directions,” but this is also the case for features in complex shapes and is a challenge that has to be addressed

\*FO = fiber orientation, FLD = fiber length distribution, EMTA = Eshelby-Mori-Tanaka Approach, D-LFT = D-LFT Pushtrusion®

# Collaborator Contributions

- ▶ **PNNL (Lead)** : Predictive engineering tool development
- ▶ **Toyota** : Complex part mold, Body system analysis
- ▶ **Magna** : Complex part molding, Cost analysis
- ▶ **PlastiComp** : LCFT compounding, Plaque and complex part molding, Cost analysis
- ▶ **Autodesk** : Rheological/physical property characterization, Process model improvement
- ▶ **University of Illinois** : Model / process consulting
- ▶ **Purdue** : Fiber orientation & length measurement
- ▶ **Virginia Tech** : Fiber orientation & length measurement

# Remaining Challenges/Barriers

- ▶ Predicting FO accurately at all locations in a complex shape
  - Challenge to model-based design of complex parts
- ▶ Accurate/automated method for FLD experimental measurement
  - Challenge to assessment of model prediction
- ▶ Injection molding of high LCF fiber loading that fills the mold, retains fiber length, and achieves well-dispersed fibers
  - Challenge to optimized part thickness/performance
- ▶ Cost of carbon fiber and molding process
  - Challenge cost competitiveness of process
  
- ▶ Prediction of mechanical performance (i.e. strength, crashworthiness, fatigue endurance, etc.) from material and process parameters
  - Barrier to broader use of LCFTs in vehicle body system

\* FO = Fiber orientation, FLD = fiber length distribution, LCFT = long carbon fiber thermoplastic composite

# Proposed Future Research

Project Complete

## Opportunities for Future Investment:

Injection Molding → Compression Molding

- ▶ Extend Predictive Engineering Tools Validated for injection-molded long-carbon fiber thermoplastic composites to compression-molded chopped carbon-fiber thermoplastic composites

Stiffness Based Design → Strength Based Design

- ▶ Develop predictive tools for strength and impact strength based on material/molding parameters (requires understanding non-linear behavior of the polymer and of fiber/matrix interfaces resulting from molding conditions and parameters)

# Summary Slide

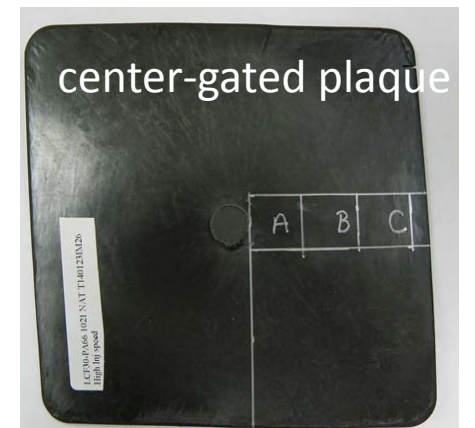
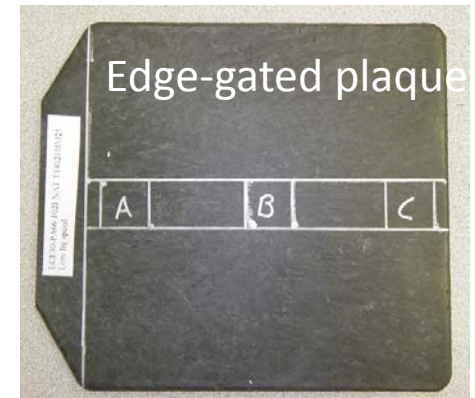
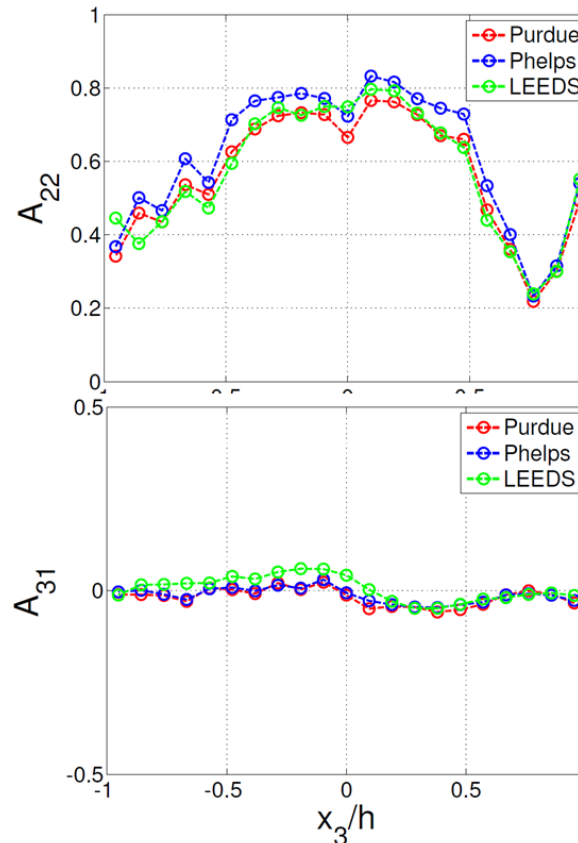
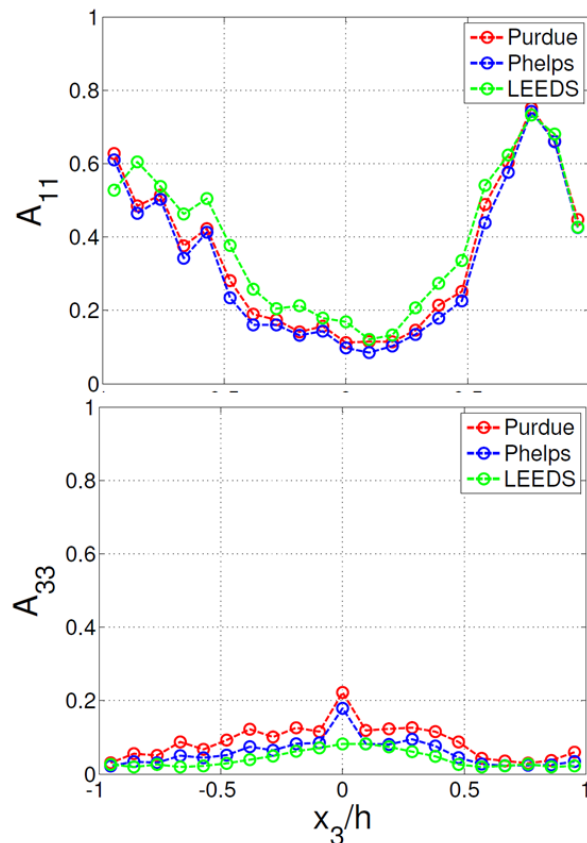
- ▶ Previously developed engineering tools were optimized and validated to successfully predict fiber orientation (FO) and length distribution (FLD) in complex 3D automotive parts injection molded from long carbon fiber-reinforced polypropylene and polyamide-6,6 compounds
- ▶ Using computed resulting moduli as criteria, the validated tools successfully predicted fiber length distribution within 15% of measured data in all cases and fiber orientation within 15% of measured data in 88% of cases.
- ▶ Technology used in the 50%LCF/PA66 part considered is estimated to have the potential for 22% weight savings for the body vehicle system at a cost of 5 times the \$3.18 per pound saved DOE target.
- ▶ Development of similar engineering tools to predict additional processes such as compression molding and additional attributes such as impact strength is expected to enable design for increase weight saving opportunities.

# Technical Back-Up Slides



# Fiber Orientation Measurements on Plaques

- **Purdue** developed and validated a fiber orientation measurement method based on the principles of the method developed by University of Leeds
- Applied to measure FO on **PlastiComp** plaques at selected locations A, B, and C



# Validation of Fiber Length Predictions for Plaques (cont.)

- ▶ The 15% accuracy criterion based on calculated moduli has been met for all the cases for plaques

Results illustrated for the slow-fill 30wt% LCF/PA66 edge-gated plaque

Tensile Modulus	$E_{11}$ (mid-plane FLD) MPa	$E_{11}$ (3D FLD) MPa	$E_{11}$ (measured FLD) MPa	Agreement between measured and 3D
Loc. A	22499	22363	22309	0.24%
Loc. B	25500	25313	25427	0.45%
Loc. C	26310	26127	26106	0.08%
Tensile Modulus	$E_{22}$ (mid-plane FLD) MPa	$E_{22}$ (3D FLD) MPa	$E_{22}$ (measured FLD) MPa	Agreement between measured and 3D
Loc. A	24620	24469	24480	0.04%
Loc. B	19802	19666	19729	0.32%
Loc. C	19123	19001	18987	0.07%
Flexural Modulus	$D_{11}$ (mid-plane FLD) MPa.mm <sup>3</sup>	$D_{11}$ (3D FLD) MPa.mm <sup>3</sup>	$D_{11}$ (measured FLD) MPa.mm <sup>3</sup>	Agreement between measured and 3D
Loc. A	86813	86293	86085	0.24%
Loc. B	86750	86137	86511	0.43%
Loc. C	88210	87622	87556	0.08%
Flexural Modulus	$D_{22}$ (mid-plane FLD) MPa.mm <sup>3</sup>	$D_{22}$ (3D FLD) MPa.mm <sup>3</sup>	$D_{22}$ (measured FLD) MPa.mm <sup>3</sup>	Agreement between measured and 3D
Loc. A	56729	56437	56320	0.21%
Loc. B	53404	53090	53282	0.36%
Loc. C	51807	51525	51493	0.06%

# Validation of Fiber Length Predictions for Complex Parts (cont.)

- The 15% accuracy of calculated moduli criterion was met for all the cases

## Results illustrated for the 30wt% LCF/PA66 ribbed part

Modulus (Location A)	Using Predicted FLD	Using Measured FLD	Agreement within	Modulus (Location B)	Using Predicted FLD	Using Measured FLD	Agreement within
$E_{11}$ (MPa)	23602	23898	1.24%	$E_{11}$ (MPa)	29761	29589	0.58%
$E_{22}$ (MPa)	16377	16558	1.09%	$E_{22}$ (MPa)	11896	11848	0.41%
$D_{11}$ (MPa.mm <sup>3</sup> )	57882	58595	1.22%	$D_{11}$ (MPa.mm <sup>3</sup> )	71669	71261	0.57%
$D_{22}$ (MPa.mm <sup>3</sup> )	30812	31103	0.94%	$D_{22}$ (MPa.mm <sup>3</sup> )	19902	19849	0.27%

Modulus (Location C)	Using Predicted FLD	Using Measured FLD	Agreement within	Modulus (Location D)	Using Predicted FLD	Using Measured FLD	Agreement within
$E_{11}$ (MPa)	34243	34139	0.31%	$E_{22}$ (MPa)	18589	17783	4.53%
$E_{33}$ (MPa)	9508	9492	0.17%	$E_{33}$ (MPa)	18727	17907	4.58%
$D_{11}$ (MPa.mm <sup>3</sup> )	74321	74100	0.30%	$D_{22}$ (MPa.mm <sup>3</sup> )	3737	3584	4.27%
$D_{33}$ (MPa.mm <sup>3</sup> )	19968	19939	0.15%	$D_{33}$ (MPa.mm <sup>3</sup> )	3926	3762	4.36%

Measured FODs at the respective locations were used in the computations

# Resources

## ► Project Complete

## ► Resources proposed: \$2.1M

- DOE: \$1.0M
- Cost share: \$1.1M (52%)

## ► Resources received: \$2.4M

- DOE: \$1.0M (received FY12)
- Cost share: \$1.4M (58%) (through FY16)
  - Autodesk, Toyota, Magna, PlastiComp, Purdue

